LA-UR- 99- 6076

c./

Approved for public release; distribution is unlimited.

Title: Technical Description of Computational Problems in the Intercomparison of 3D Radiation Codes (I3RC)

Author(s): Anthony B. Davis,
Los Alamos National Laboratory, Space & Remote Sensing Sciences Group (NIS-2), Los Alamos, NM 87545.

Alexander Marshak, and Robert F. Cahalan
NASA's Goddard Space Flight Center, Climate & Radiation Branch (Code 913), Greenbelt, Md 20771.

Submitted to: Proceedings of Intercomparison of 3-dimensional Radiation Codes: I3RC-99 - First Workshop: 17 - 19 November, 1999, Tucson, AZ
Extended Abstract

Los Alamos
NATIONAL LABORATORY

TECHNICAL DESCRIPTION OF COMPUTATIONAL PROBLEMS IN THE INTERCOMPARISON OF 3D RADIATION CODES (I3RC)

Anthony B. Davis,† Alexander Marshak,‡ and Robert F. Cahalan‡

†*Los Alamos National Laboratory, Space & Remote Sensing Sciences Group (NIS-2), Los Alamos, NM 87545.*
‡*NASA's Goddard Space Flight Center, Climate & Radiation Branch (Code 913), Greenbelt, Md 20771.*

Outline

We describe in unambiguous mathematical detail the computational problems of interest to the Intercomparison of 3D Radiation Codes (I3RC), Phase I. In section 1, the dependent and independent variables of the 3D radiative transfer equation (RTE) are defined and the I3RC problems are set-up through the specification of boundary conditions, or an internal source-term, and the main difficulty in computational radiative transfer is traced to the multiple scattering term in the RTE. In section 2, the required output quantities are defined and related to the Independent Pixel Approximation (IPA) which is in essence the starting point of I3RC. Section 3 describes how the input (extinction) and output (radiation) fields for the 3 test-cases are specified numerically and section 4 summarizes the choices of optical and illumination parameters, case-by-case.

1. Setting Up the General 3D Albedo Problem for Numerical Solution

We are given an open 3D domain $M = (0,L_x)\otimes(0,L_y)\otimes(0,L_z)$ which represents an optical medium with a spatially variable (total) extinction $\sigma(\boldsymbol{r})$ with $\boldsymbol{r} = (x,y,z)^{\mathrm{T}}$ where superscript "T" means transpose. We will assume here spatially uniform single-scattering albedo ϖ_0 and phase function $p(\Omega\bullet\Omega')$ where $\Omega^{(\prime)}$ is the unit-vector indicating propagation direction after (before) a scattering event. We wish solve the steady-state integro-differential RTE [*Chandrasekhar*, 1950]

$$\nabla\bullet I = -\sigma(\boldsymbol{r})I(\boldsymbol{r},\Omega) + \varpi_0\sigma(\boldsymbol{r})\int p(\Omega'\bullet\Omega)I(\boldsymbol{r},\Omega)\mathrm{d}\Omega' + S(\boldsymbol{r},\Omega) \tag{1}$$

for $I(\boldsymbol{r},\Omega)$ where $\boldsymbol{r} \in \underline{\mathrm{M}}$, the "closure" of the open set M, and $\|\Omega\| = \sqrt{\Omega^2} = \sqrt{\Omega\bullet\Omega} = 1$; $S(\boldsymbol{r},\Omega)$ designates an internal source term. We will represent the unit vector $\Omega = (\Omega_x,\Omega_y,\Omega_z)^{\mathrm{T}}$ in polar coordinates; so $\Omega_x = \eta\cos\varphi$, $\Omega_y = \eta\sin\varphi$, $\Omega_z = \mu$ ($\eta = \sqrt{1-\mu^2}$) where $\theta = \cos^{-1}\mu$ and φ are the usual polar angles. The phase function has been assumed azimuthally symmetric and is normalized so that $\int p(\Omega'\bullet\Omega)\mathrm{d}\Omega = 1$ where $\mu_s = \Omega'\bullet\Omega$ is the cosine of the scattering angle and $\mathrm{d}\Omega = 2\pi\mathrm{d}\mu_s$. Physically, this means the scatterers are either spherical (like cloud droplets) or randomly oriented. Extinction $\sigma(\boldsymbol{r})$, also assumed independent of direction of propagation, is related to the photon mean free path (MFP) $\lambda = 1/\sigma$ which, importantly, is a local quantity in 3D radiative transfer. These optical properties are dependent on the density of scatterers and their cross-sections for scattering and absorption, appropriately averaged over the droplet population. Similarly, $p(\mu_s)$ is related to the population averaged differential cross-section for scattering; an important parameter of the phase function is the asymmetry factor $g = 2\pi\int\mu_s p(\mu_s)\mathrm{d}\mu_s$.

This solution is uniquely defined as soon as we specify $S(\boldsymbol{r},\Omega)$ and the boundary conditions (BCs) for $I(\boldsymbol{r},\Omega)$ on $\partial\mathrm{M} = \underline{\mathrm{M}}\backslash\mathrm{M}$. In the I3RC study, we are interested in so-called "albedo" problems where $S(\boldsymbol{r},\Omega) \equiv 0$ in Eq. (1) and $\theta_0 = \cos^{-1}\mu_0$ is the solar zenith angle ($\varphi_0 = \pi$ in I3RC conventions): for $(x,y)^{\mathrm{T}} \in (0,L_x)\otimes(0,L_y)$, we set

$$I(x,y,L_z,\Omega) = F_0\delta(\Omega+\Omega_0),\ \Omega_z < 0, \tag{2a}$$

where F_0 is the solar constant, and

$$I(x,y,0,\Omega) = 0,\ \Omega_z > 0, \tag{2b}$$

in absence of surface reflection, or

$$\pi I(x,y,0,\Omega) = \alpha \int_{\Omega'_z\leq 0} |\Omega_z'|I(x,y,0,\Omega')\mathrm{d}\Omega',\ \Omega_z > 0, \tag{2b'}$$

for a Lambertian surface with spatially uniform albedo α; in the horizontal, we use cyclical BCs,

$$I(L_x,y,z,\Omega) = I(0,y,z,\Omega),\ \forall\Omega, \tag{2c}$$

for $(y,z)^T \in (0,L_y)\otimes(0,L_z)$, and similarly in $(0,L_x)\otimes(0,L_z)$. Figure 1 illustrates the geometry and notations.

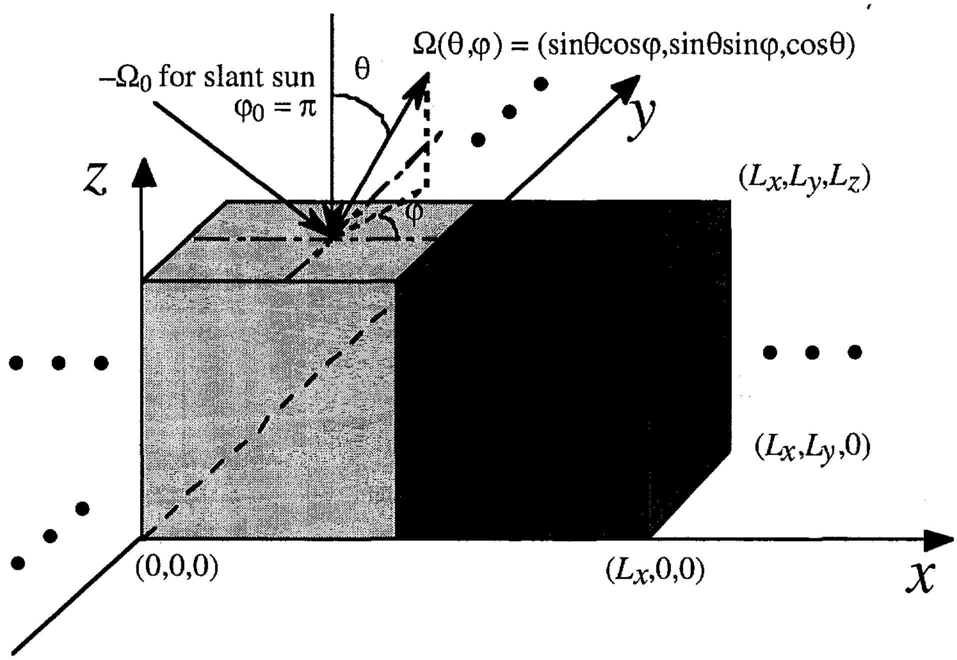

Figure 1: *Schematic of Albedo Problem Illustrated with Square-Wave Cloud Model (Case #1).* In absence of y-variability, grid size in this direction, L_y, is arbitrarily set equal to its counterpart for z, $L_z = 0.25$ km $= \ell_x = L_x/2$ ($N_x = 2$). Infinite periodic replication of the basic element in the picture is represented by "···" (x-direction) and "⋰" (y-direction). Both zenith and slant solar illuminations are shown along with an arbitrary reflected beam.

One can also use $I(\boldsymbol{r},\Omega)$ to model only the "diffuse" component of the radiance field:

$$I(\boldsymbol{r},\Omega) \text{ becomes } I(\boldsymbol{r},\Omega) + F_0\delta(\Omega+\Omega_0)\exp[-\tau(\boldsymbol{r};\boldsymbol{r}_0(\boldsymbol{r},\Omega_0))] \tag{3}$$

where the latter term is the "direct" (or "non-scattered" or "un-collided") component with

$$\boldsymbol{r}_0(\boldsymbol{r},\Omega_0) = \boldsymbol{r} + \Omega_0 s_0,\ s_0 = (L_z-z)/\Omega_{0z} \tag{4}$$

being the piercing point at the upper (illuminated) boundary, $z = L_z$, for the solar beam reaching $\boldsymbol{r}$. We also need to define

$$\tau(\boldsymbol{r};\boldsymbol{r}') = \int_0^{\|\boldsymbol{r}'-\boldsymbol{r}\|} \sigma(\boldsymbol{r}+s(\boldsymbol{r}'-\boldsymbol{r})/\|\boldsymbol{r}'-\boldsymbol{r}\|)\mathrm{d}s \tag{5}$$

as the optical distance between two points in $\underline{\mathrm{M}}$. In this case, we set $I(x,y,L_z,\Omega) = 0$ in the upper BC in (2a) and, in the RTE (1), we use the following internal source term:

$$S(\boldsymbol{r},\Omega) = F_0\exp[-\tau(\boldsymbol{r};\boldsymbol{r}_0(\boldsymbol{r},\Omega_0))]\sigma(\boldsymbol{r})\varpi_0 p(-\Omega\bullet\Omega_0). \tag{6}$$

REMARKS:

a. Formal Solution of RTE.

In absence on scattering ($\varpi_0 = 0$), the 3D RTE is integrable in closed form:

$$I(\boldsymbol{r},\Omega) = \int_0^{s_{\partial\mathrm{M}}(\boldsymbol{r},\Omega)} S(\boldsymbol{r}-s\Omega,\Omega)\exp[-\tau(\boldsymbol{r}-s\Omega;\boldsymbol{r})]\mathrm{d}s \tag{7}$$

where $s_{\partial\mathrm{M}}(\boldsymbol{r},\Omega)$ defines the boundary piercing point for the beam arriving at $\boldsymbol{r}$ in direction Ω which can be computed much as in Eq. (4). Note that Ω is clearly more like a parameter or label for the radiance field than an independent variable. This no-scattering assumption is often justifiable in thermal IR and microwave spectral regions where, furthermore, $S(\boldsymbol{r},\Omega)$ is $(1-\varpi_0)\sigma(\boldsymbol{r})$

times Planck's function, hence isotropic (does not depend explicitly on Ω). As an example of an anisotropic source term, formally using (6) in (7) leads to a 1st-order scattering approximation in the solution of the RTE. In fact, one can interpret $S(\boldsymbol{r},\Omega)$ in Eq. (7) as the (Ω-integral) multiple scattering source term in the RTE which leads to the integral form of the RTE spelled out in Eq. (11–13) below.

b. Expansion in Spherical Harmonics.

As soon as $\varpi_0 > 0$, the RTE in (1) is mathematically speaking an infinite system of coupled 1st-order PDEs with its dependent variables' labels, its coefficients and BCs determined by angular variables. The complexity of this situation can be greatly reduced by noting that the angular coupling in Eq. (1) is actually to a convolution product of $p(\Omega'\bullet\Omega)$ and $I(\boldsymbol{r},\Omega)$ in the spherical coordinates of Ω, so the angular coupling becomes merely tri-diagonal for the spherical-harmonic decompositions of $p(\Omega'\bullet\Omega)$ and $I(\boldsymbol{r},\Omega)$, respectively, p_l and $I_{lm}(\boldsymbol{r})$ with $l \geq 0$ ($|m| \leq l$). Many numerical approaches exploit this simplification, including DANTSYS [*Davis et al.*, 1999; and references therein] and SHDOM [*Evans*, 1998]. The first two spherical harmonics have a special significance: at $m = 0$ we find a scalar measure of radiant energy (or photon) density,

$$J(\boldsymbol{r}) = \int I(\boldsymbol{r},\Omega)\mathrm{d}\Omega, \tag{8}$$

and at $m = 1$ we find the radiant energy flux vector,

$$\boldsymbol{F}(\boldsymbol{r}) = \int \Omega I(\boldsymbol{r},\Omega)\mathrm{d}\Omega. \tag{9}$$

Radiant energy conservation is expressed by

$$\nabla\bullet\boldsymbol{F} + (1-\varpi_0)\sigma(\boldsymbol{r})J(\boldsymbol{r}) = 0, \tag{10}$$

obtained by integrating over all angles the RTE in (1) when $S(\boldsymbol{r},\Omega) \equiv 0$. Diffusion theory [*Davis et al.*, 1999; and references therein] uses only the quantities in (8–9) in Eq. (10), which is exact, and an approximate relation between $\boldsymbol{F}$ and J (Fick's law).

c. Integral Form of RTE.

Another conceptual simplification is to transform the angular-integral/spatially-differential RTE into a space-angle (5-dimensional) integral equation that incorporates the BCs. For the 3D atmospheric albedo problem with an absorbing surface, we have [*Marchuk et al.*, 1980]

$$I(\boldsymbol{r},\Omega) = \int_{\mathrm{M}} \int_{4\pi} K[\boldsymbol{r}',\Omega';\boldsymbol{r},\Omega]\, I(\boldsymbol{r}',\Omega')\; \mathrm{d}\boldsymbol{r}'\mathrm{d}\Omega' + f(\boldsymbol{r},\Omega), \tag{11}$$

where the propagation kernel is given by

$$K[\boldsymbol{r}',\Omega';\boldsymbol{r},\Omega] = \varpi_0\, \sigma(\boldsymbol{r}')\, p(\Omega'\bullet\Omega)\, \frac{\exp[-\tau(\boldsymbol{r}';\boldsymbol{r})]}{\|\boldsymbol{r}-\boldsymbol{r}'\|^2}\, \delta\Big(\Omega - \frac{\boldsymbol{r}-\boldsymbol{r}'}{\|\boldsymbol{r}-\boldsymbol{r}'\|}\Big) \tag{12}$$

and the new source term is

$$f(\boldsymbol{r},\Omega) = \int_{\mathrm{M}} K[\boldsymbol{r}',\Omega_0;\boldsymbol{r},\Omega]\, \exp[-\tau(\boldsymbol{r}';\boldsymbol{r}_0)]\; \mathrm{d}\boldsymbol{r}'. \tag{13}$$

The above integral form of the RTE underscores the nonlocal nature of the multiple scattering problem. Equations (11–13) and their kin are exploited numerically in several methods, including SHDOM and Monte Carlo (at least when local estimation techniques are invoked).

d. Green's Functions and Superposition Principle.

The RTE in (1) is linear with respect to the sources, internal and/or at boundaries. This leads to a superposition principle that can be used to express the solution of the general "3D atmosphere over Lambertian surface problem" (or any other for that matter) to an infinite weighted sum of fundamental solutions, or Green's functions, defined by $S(\boldsymbol{r},\Omega) = \delta(\boldsymbol{r}-\boldsymbol{r}^*)\delta(\Omega-\Omega^*)$ and homogeneous BCs (i.e., no incoming radiation). "Backward" Monte Carlo techniques [*Marchuk et al.*, 1980; *Marshak and Davis*, 1999] exploit this formalism to give accurate numerical estimates of single radiance values (in this case, at point $\boldsymbol{r}^*$ in direction Ω^*) for one or more source geometries; this is one of the most efficient ways of modeling a single instrument's response.

2. Definitions of 2D σ- and I-Related Quantities Relevant to I3RC – Phase 1

For I3RC, we are interested primarily in the "escaping" radiance fields, namely,

$$I(x,y,L_z,\Omega) \text{ with } \Omega_z \geq 0, \tag{14a}$$

$$I(x,y,0,\Omega) \text{ with } \Omega_z \leq 0, \tag{14b}$$

for $(x,y)^T \in (0,L_x)\otimes(0,L_y)$, respectively for reflected and transmitted radiation. Of particular interest to cloud remote sensing applications from space and ground are vertical radiances, respectively towards zenith and towards nadir; these quantities are usually expressed in non-dimensional "bidirectional reflection distribution function" (BRDF) units as a ratio of I with $\mu_0 F_0/\pi$, the radiance from a perfect Lambertian reflector, specifically:

$$I\uparrow(x,y) = \pi I(x,y,L_z,\ 0,0,1))\ /\ \mu_0 F_0, \tag{15a}$$

$$I\downarrow(x,y) = \pi I(x,y,0,\ 0,0,-1))\ /\ \mu_0 F_0. \tag{15b}$$

In radiative energy budget applications, one is more interested in normalized hemi-spherical fluxes at boundaries:

$$R(x,y) = \int_{\Omega_z \geq 0} \Omega_z I(x,y,L_z,\Omega)\mathrm{d}\Omega\ /\ \mu_0 F_0, \tag{16a}$$

$$T(x,y) = \int_{\Omega_z \leq 0} |\Omega_z| I(x,y,0,\Omega)\mathrm{d}\Omega\ /\ \mu_0 F_0, \tag{16b}$$

which are respectively the albedo and transmittance fields (not vertical components of net fluxes). Note that, if the direct/diffuse separation in (3) in invoked, the directly transmitted contributions are required in (14b), possibly in (15b), and certainly in (16b) as well as in (2b') where $T(x,y)$ appears on the right hand side and (10).

Another quantity of interest is "apparent" column absorption,

$$A_{\mathrm{app}}(x,y) = [-F_z(x,y,L_z)+F_z(x,y,0)]\ /\ \mu_0 F_0 = 1 - R(x,y) - (1-\alpha)T(x,y), \tag{17}$$

as well as (true) column absorption,

$$A(x,y) = (1-\varpi_0)\int_0^{L_z} \sigma(\boldsymbol{r})J(\boldsymbol{r})\mathrm{d}z\ /\ \mu_0 F_0 = -\int_0^{L_z} \nabla\bullet\boldsymbol{F}(\boldsymbol{r})\mathrm{d}z\ /\ \mu_0 F_0, \tag{18}$$

where $-\nabla\bullet\boldsymbol{F}(\boldsymbol{r})$ is proportional to the local solar heating rate. The difference between the apparent and true absorptions in Eqs. (17–18) is the vertically-integrated horizontal flux divergence:

$$H(x,y) = 1 - A(x,y) - R(x,y) - (1-\alpha)T(x,y) = \int_0^{L_z} [\partial_x F_x + \partial_y F_y]\mathrm{d}z\ /\ \mu_0 F_0. \tag{19}$$

Note that in typical 3D geometries H can be quite small even though none of its positive (A, R, T) or signed (A_{app}, F_x, F_y) components are.

Although generally insufficient to describe the 3D structure of a real cloud, often all that is available from remote sensing data (cf. I3RC "Landsat" case) or simple stochastic models (such as bounded cascades [*Cahalan et al.*, 1994a]) is optical depth as a function of position in the horizontal plane, i.e.,

$$\tau^*(x,y) = \tau(x,y,0;x,y,L_z) \tag{20}$$

from Eq. (5) for $(x,y)^T \in (0,L_x)\otimes(0,L_y)$. In the independent pixel approximation (IPA) to 3D radiative transfer, all horizontal fluxes are explicitly ignored so Eq. (19) vanishes identically and $\tau^*(x,y)$ is all that is needed to predict the other fields. The I3RC study is focused entirely on deviations from the IPA, locally and over the entire (x,y)-domain which *Cahalan et al.* [1994a,b] call the "IPA bias."

3. Numerical Specification of σ- and *I*-Variabilities for I3RC – Phase 1

In the simplest cases, the extinction field $\sigma(\boldsymbol{r})$ can specified analytically, e.g., I3RC case #1 or "square-wave" cloud (see Fig. 1):

$$\sigma(\boldsymbol{r}) = [10 + 8\times\mathrm{sign}(x-L_x/2)]\,/L_z \qquad (21)$$

where $L_x = 0.5$ km, $L_z = 0.25$ km and, formally, $L_y = \infty$. More generally, it is specified on a grid, e.g., I3RC cases #2 and #3: "MMCR" cloud (see Fig. 2) and "Landsat" cloud (see Fig. 3). Either way, the radiance field will necessarily be given numerically on a spatial grid, so we need to specify grid sizes on all three axes; in summary:

axis:	x	y	z
grid size (integer):	N_x	N_y	N_z
outer scale:	L_x	L_y	L_z
grid constant:	$\ell_x = L_x/N_x$	$\ell_y = L_y/N_y$	$\ell_z = L_z/N_z$
BCs:	cyclic, Eq. (2c)	cyclic	(2a) and (2b) or (2b')

The I3RC σ-grids are characterized as follows:

I3RC case	name	N_x	L_x (km)	N_y	L_y (km)	N_z	L_z (km)	cell-size $\ell_x\times\ell_y\times\ell_z$ (m)
#1	square-wave	2¶	0.50	1	∞	1	0.25	250×∞×250
#2	MMCR	640	32	1	∞	54	2.43	50×∞×45
#3	Landsat	128	3.8	128	3.8	≥1◊	2.4&	30×30×var.

¶The ± deviations have equal length and $N_x = 32$ ($\ell_x = 15.6$ m) is actually for the required radiation fields, the *I*-grid.
◊Enough to capture the cloud height variability in methods that require a regular 3D grid. &Maximum cloud height.

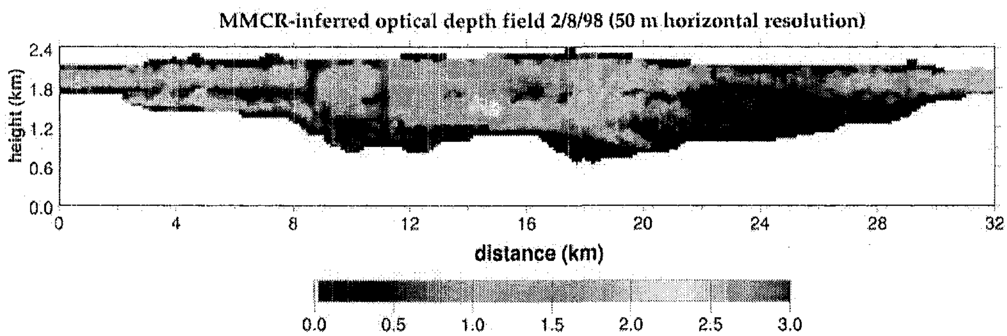

Figure 2: *MMCR Cloud Model (Case #2).* The gray scale refers to cell optical depth, $\sigma(\boldsymbol{r})\ell_z$.

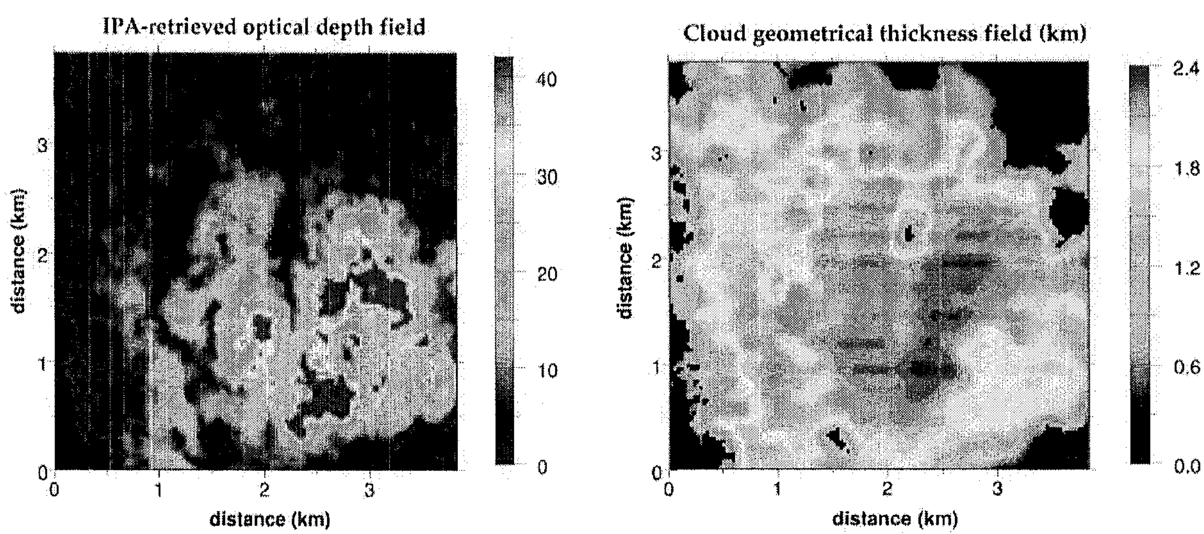

Figure 3: *Landsat Cloud (Case #3).* Optical depth (left) and physical thickness (right) fields.

Although not a requirement in general, the grids for σ and I (and related quantities defined in section 2) are identical in I3RC. Sub-grid scale assumptions on σ and I depend on the specific method of solution and its implementation; constant (or averaged) is the standard in Monte Carlo methods, linear or bi-linear variation are the most common when the RTE is spatially discretized.

4. Parameter Space Explored in I3RC – Phase 1

In computational problem set-up in sections 1 and 3, we have left only a few parameters unspecified. They are on the one hand solar zenith angle $\theta_0 = \cos^{-1}\mu_0$ and surface reflectance α for BCs and, on the other hand, the optical (scattering/absorption) properties defined by single-scattering albedo ϖ_0 along with the specific choice of phase function $p(\mu_s)$. This last choice is restricted to either an academic *Henyey-Greenstein* [1941] model,

$$p(\mu_s) = \frac{1}{4\pi}(1-g^2)/[1+g^2-2g\mu_s]^{3/2} \tag{22}$$

with asymmetry factor $g = 0.85$ or a more realistic *Deirmendjian* [1969] "C1" model. The following table summarizes the numerical experiments in I3RC:

Case #	$\mu_0 = 1$	$\mu_0 = 0.5$	$\alpha = 0$	$\alpha = 0.4$	$\varpi_0 = 1$	$\varpi_0 = 0.99$	p.f.=HG	p.f.=C1
1	√		√		√		√	
1		√	√		√		√	
1	√		√			√	√	
1		√	√			√	√	
2	√		√		√		√	
2		√	√		√		√	
2	√		√			√	√	
2		√	√			√	√	
2		√		√	√		√	
2	√		√		√			√
2		√	√		√			√
2		√	√		√			√
3	√		√		√		√	
3		√	√		√		√	
3	√		√			√	√	
3		√	√			√	√	

References

Cahalan, R.F., W. Ridgway, W.J. Wiscombe, T.L. Bell, and J.B. Snider, 1994: The albedo of fractal stratocumulus clouds, *J. Atmos. Sci.*, **51**, 2434–2455.

Cahalan, R.F., W. Ridgway, W.J. Wiscombe, S. Gollmer, and Harshvardhan, 1994: Independent pixel and Monte Carlo estimates of stratocumulus albedo, *J. Atmos. Sci.*, **51**, 3776–3790.

Chandrasekhar, S., 1950: *Radiative Transfer*, Oxford University Press, reprint by Dover, 1960, New York (NY).

Davis, A.B., D.E. Kornreich, Z. Qu, and C.E. Rohde, 1999: Diffusion-Based Approximations to the 3D Radiative Transfer Equation, its Reduction to Discrete Ordinates, and Discrete-Angle Formulations, in *Proceedings of International Workshop on Intercomparison of 3D Radiation Codes – Phase I*, this volume.

Deirmendjian, D., 1969: *Electromagnetic Scattering on Spherical Polydispersions*, Elsevier, New York (NY).

Evans, K.F., 1998: The Spherical Harmonics Discrete Ordinate Method for Three-Dimensional Atmospheric Radiative Transfer, *J. Atmos. Sci.*, **55**, 429–446.

Henyey, L.C., and J.L. Greenstein, 1941: Diffuse radiation in the galaxy, *Astrophys. J.*, **93**, 70–83.

Marshak, A., and A.B. Davis, 1999: *Monte Carlo Solution of the Radiative Transfer Equation in Clouds – Some Formalism*, tutorial document (in preparation).

Marchuk, G., G. Mikhailov, M. Nazaraliev, R. Darbinjan, B. Kargin, and B. Elepov, 1980: *The Monte Carlo Methods in Atmospheric Optics*, Springer-Verlag, New-York (NY).